Discussion Session II

NIST Role in Combinatorial Informatics Research and Standards Development

NCMC-3
May 22, 2003
NIST

NIST
Combinatorial
Methods Center

Discussion I Summary:

Elements Committee

- What is the Aim?
  - Instrument Control?†
  - Standard Output?*
- What is the scope?
  Who's problems are we solving?
  - Combi informatics vs age-old information issues
  - Success in starting small
  - A timely success (even small)
  - A minimal set of elements
- "The List" of positive attributes
  - *† Transparency on both ends
  - Extensibility
  - Long-term storage/retrieval
  - Measurement Validation

Exploratory Committee

- "Market Research" Effort
  - Identify target vendors
  - "Value Proposition" to vendors
  - Vendor outreach --> LRIG
- Opportunities for Leverage
  "We shouldn't start from scratch!"
  - What does pharma offer?
  - *XML efforts and schema
  - "Onion Skin" approach
  - Other Combi Communities
    Europe and Asia?
  - †Is Active-X a solution (if it were ubiquitous)? Can we help make it so?

What we require to for further action:

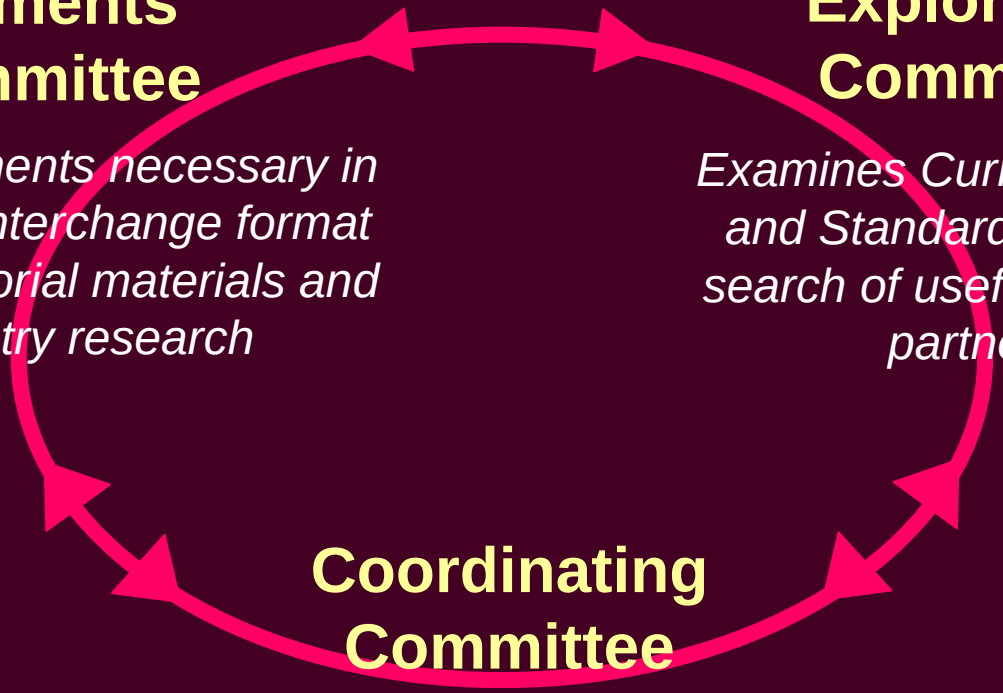
Commitment to a Working Group

- Justification/planning of Next Steps
  - Funding for formal processes
- A coherent message for vendors

Given a Working Group (i.e. a first success):

- Regular discussions via e-avenues
- A Breakout Session at NCMC-4 (Fall 2003)

Proposed Working Group Structure



Elements Committee

Defines elements necessary in a standard interchange format for combinatorial materials and chemistry research

Exploratory Committee

Examines Current Formats and Standards Efforts in search of useful ideas and partners.

Coordinating Committee

Coordinates Efforts
Defines Next-Steps
Seeks Funding

Our Panel:

David Evans
Chairman, Laboratory Robotics Interest Group – Chesapeake Chapter

David Rothman
Dow Chemical Company

Laurel Harmon
Striatus Inc.

Kapeel Krishana
Rhodia Inc.

John Barkley
Software Diagnostics and Conformance Testing Division, NIST

Barbara Guttman
Software Diagnostics and Conformance Testing Division, NIST

Facilitators

Eric Amis
Chief, Polymers Division, NIST

Michael Fasolka
Polymers Division, NIST

Cher Davis
Technical Coordinator, NCMC

Stephen Mumby
Accelrys

Goals of this Discussion (and Discussion II):

1. **Begin a process for the development of data interchange standards for combinatorial research**
    - Form a *Combinatorial Materials Research Data Standards Working Group* aimed at defining necessary interchange data file elements and structures (e.g. XML tags/descriptors).
    - If possible, commit in principle to an interchange data standard for combi materials research that is XML-based.
2. **Outline industrial needs for combinatorial informatics**
    - Avenues for NIST research on information tools (e.g. statistical techniques)

What will the Working Group do?

First, we must answer the following:

What do we want from a data standard?

What do we mean by “combi data interchange standard?”

What elements are necessary for making such a standard useful?

What have other efforts accomplished?

Are there useful structures that we can adopt/combine?

Let’s not start from scratch!

What can we agree on?

- Working Group Formation?
- Working Group Structure?
- XML?
- More?